Nonlocality and entanglement in the XY model

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Nonlocality and quantum entanglement constitute two special features of quantum systems of paramount importance in quantum information theory (QIT). Essentially regarded as identical or equivalent for many years, they constitute different concepts. Describing nonlocality by means of the maximal violation of two Bell inequalities, we study both entanglement and nonlocality for two and three spins in the XY model. Our results shed a new light into the description of nonlocality and the possible information-theoretic task limitations of entanglement in an infinite quantum system.

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Schrödinger 's reply [1] to the paradox posed by Einstein, Podolsky and Rosen (EPR) [2] motivated the modern notion of entanglement in a quantum system. EPR suggested a description of nature, called "local realism", which assigned independent properties to distant parties of a composite physical system, to conclude that QM was an incomplete theory. Schrödinger, instead, did not recognise such conflict and regarded entanglement as *the* characteristic feature of QM.

The most significant progress toward the resolution of the EPR debate was made by Bell [3]. Bell showed that local realism, in the form of local variable models (LVM), implied constraints on the predictions of spin correlations, known as Bell inequalities. Spatially separated observers sharing an entangled state and performing measurements on them may induce (nonlocal) correlations which cannot be simulated by local means (violate Bell inequalities). This limitation to our physical understanding is nowadays exploited for implementing information-theoretic tasks.

Ever since Bell's contribution, entanglement and nonlocality were essentially identified as the same thing. With the advent QIT, interest in entanglement dramatically increased over the years for it lies at the basis of several important processes and applications which possess no classical counterpart [4, 5].

Confusion between nonlocality and entanglement arose when the usefulness of quantum correlations was put in doubt (see [6]). The nonlocal character of entangled states was clear for pure states since all entangled pure states of two qubits violate the CHSH inequality and are therefore nonlocal (*Gisin's theorem*) [7]. However, the situation became more involved when Werner [8] discovered that while entanglement is necessary for a state to be nonlocal, for mixed states is not sufficient.

Entanglement is commonly viewed as a useful resource for various information-processing tasks. Yet, there exist certain procedures, such as device-independent quantum key distribution [9] and quantum communication complexity problems [10], which can only be carried out provided the corresponding entangled states exhibit nonlocal correlations. Therefore we are naturally led to the question whether nonlocality and entanglement constitute two different resources.

The purpose of the present work is to shed some light upon the relation between entanglement and nonlocality, through the maximal violation of a Bell inequality, in an infinite system, namely, the XY model [11] .

The model Hamiltonian of the anisotropic one-dimensional spin-$\frac{1}{2}$ XY model in a transverse magnetic field h for N particles is given by

$$H=\sum_{i=1}^{N}[(1+\gamma)S_x^jS_x^{j+1}+(1-\gamma)S_y^jS_y^{j+1}]-h\sum_{i=1}^{N}S_x^j, \quad (1)$$

where $\sigma_u^j=2S_u^j$ $(u=x,y,z)$ are the Pauli spin-$\frac{1}{2}$ operators on site j, $\gamma\in[0,1]$ and $\sigma_u^{j+N}=\sigma_u^j$. The XY model (1) for $N=\infty$ is completely solved by applying a Jordan-Wigner transformation [11, 12], which maps the Pauli (spin 1/2) algebra into canonical (spinless) fermions. This model undergoes a paramagnetic-to-ferromagnetic quantum phase transition (QPT) [13] driven by the parameter h at $h_c=1$ and $T=0$.

We will provide evidence for an anomaly that regards entanglement and nonlocality in the XY model. To such end, we will consider the correlations existing between two sites or qubits (bipartite case) and three sites or qubits (tripartite case).

Two qubits The general two-site density matrix is expressed as

$$\rho_{ij}^{(R)}=\frac{1}{4}\left[\mathbb{I}+\sum_{u,v}T_{uv}^{(R)}\sigma_u^i\otimes\sigma_v^j\right]. \quad (2)$$

$R=j-i$ indicates the distance between spins, $\{u,v\}$ denote any index of $\{\sigma_0,\sigma_x,\sigma_y,\sigma_z\}$, and $T_{uv}^{(R)}\equiv\langle\sigma_u^i\otimes\sigma_v^j\rangle$. Due to symmetry considerations, only $\{T_{xx}^{(R)},T_{yy}^{(R)},T_{zz}^{(R)},T_{xy}^{(R)}\}$ do not vanish. Barouch *et al* [12] provided exact expressions for two-point correlations, together with all the dynamics associated with an external $h(t)$. Let us consider the case where h jumps from and initial value h_0 to a final value h_f at $t=0$ (the equilibrium case is easily recovered when $h_f=h_0$) and the

$R = 1$ configuration. Following [12], one obtains that $T^{(1)}_{xx} = G_{-1}, T^{(1)}_{yy} = G_1, T^{(1)}_{zz} = G_0^2 - G_1 G_{-1} - S_1 S_{-1}$ and $T^{(1)}_{xy} = S_1$, where

$$G_R = \frac{\gamma}{\pi}\int_0^\pi d\phi \sin(R\phi)\frac{\tanh\left[\frac{1}{2}\beta\Lambda(h_0)\right]}{\Lambda(h_0)\Lambda^2(h_f)} \\ \times[\gamma^2\sin^2\phi + (h_0-\cos\phi)(h_f-\cos\phi) \\ -(h_0-h_f)(h_f-\cos\phi)\cos(2\Lambda(h_f)t)] \\ -\frac{1}{\pi}\int_0^\pi d\phi\cos(R\phi)\frac{\tanh\left[\frac{1}{2}\beta\Lambda(h_0)\right]}{\Lambda(h_0)\Lambda^2(h_f)} \\ \times\left[\{\gamma^2\sin^2\phi + (h_0-\cos\phi)(h_f-\cos\phi)\}(\cos\phi - h_f) - (h_0-h_f)\gamma^2\sin^2\phi\cos(2\Lambda(h_f)t)\right], \quad (3)$$

$$S_R = \frac{\gamma(h_0-h_f)}{\pi}\int_0^\pi d\phi\sin(R\phi)\sin\phi\frac{\sin[2\Lambda(h_f)t]}{\Lambda(h_0)\Lambda(h_f)}, \quad (4)$$

with $\Lambda(h) = [\gamma^2\sin^2\phi + (h-\cos\phi)^2]^{1/2}$. G_R is the two-point correlator appearing in the Wick theorem calculations, and $M_z = \frac{1}{2}G_0$.

Most of our knowledge on Bell inequalities and their quantum mechanical violation is based on the CHSH inequality [7]. With two dichotomic observables per party, it is the simplest nontrivial Bell inequality for the bipartite case with binary inputs and outcomes. Quantum mechanically, these observables reduce to $\mathbf{A_j}(\mathbf{B_j}) = \mathbf{a_j}(\mathbf{b_j})\cdot\sigma$, where $\mathbf{a_j}(\mathbf{b_j})$ are unit vectors in $\mathbb{R}^3$ and $\sigma = (\sigma_\mathbf{x}, \sigma_\mathbf{y}, \sigma_\mathbf{z})$ the Pauli matrices. Violation of CHSH inequality requires $Tr(\rho^{(R)}_{ij}B_{CHSH})$, that is, the expectation value of the operator B_{CHSH}

$$\mathbf{A_1}\otimes\mathbf{B_1} + \mathbf{A_1}\otimes\mathbf{B_2} + \mathbf{A_2}\otimes\mathbf{B_1} - \mathbf{A_2}\otimes\mathbf{B_2} \quad (5)$$

to be greater than 2. We shall take the optimum value over all $\{\mathbf{a_j}, \mathbf{b_j}\}$ as a proper measure for nonlocality in our state $\rho^{(R)}_{ij}$ (2). This procedure is presented in detail elsewhere [14]. Given a general two qubit state ρ in the usual computational basis, we change it into the well known Bell basis $\{|\Phi^+\rangle, |\Phi^-\rangle, |\Psi^+\rangle, |\Psi^-\rangle\}$. The ensuing matrix $\rho = \rho_\parallel + \rho_\perp$ is decomposed into two contributions, where only terms in $\rho_\parallel$

$$\begin{pmatrix} \rho_{11} & i\rho^I_{12} & i\rho^I_{13} & \rho^R_{14} \\ -i\rho^I_{12} & \rho_{22} & \rho^R_{23} & i\rho^I_{24} \\ -i\rho^I_{13} & \rho^R_{23} & \rho_{33} & i\rho^I_{34} \\ \rho^R_{14} & -i\rho^I_{24} & -i\rho^I_{34} & \rho_{44} \end{pmatrix} \quad (6)$$

contribute to $Tr(\rho B_{CHSH})$. In the XY model, state (2) is almost Bell-diagonal except for $\rho^I_{12} = \frac{1}{2}T^{(R)}_{xy}$, which is null in equilibrium ($h_f = h_0$).

Optimization is carried out and after some algebra, we obtain $2\sqrt{2}\sqrt{(\rho_{11}-\rho_{44})^2 + (\rho_{22}-\rho_{33})^2 + 4(\rho^I_{12})^2}$, with the diagonal elements of (6) arranged so that $\rho_{11} > \rho_{22} > \rho_{33} > \rho_{44}$. The specific form for our state (2) reads as

$$B^{\max}_{CHSM} \equiv \max_{\mathbf{a_j},\mathbf{b_j}} Tr(\rho^{(R)}_{ij}B_{CHSH}) = 2\sqrt{\|\mathbf{T^{(R)}}\|^2 - \min{}_{xyz} + 2\left[T^{(R)}_{xy}\right]^2}, \quad (7)$$

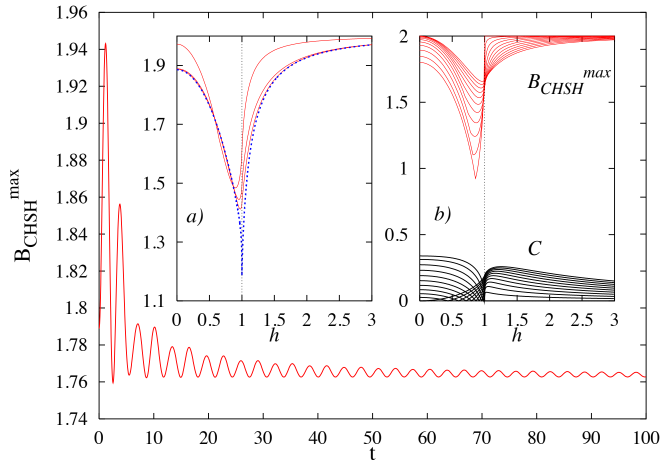

FIG. 1. (colour online). The oscillating curve depicts $B^{\max}_{CHSM}$ (7) versus time (in seconds) for $h_0 = 0.5, h_f = 0$ and $\gamma = 0.5$ for the evolved state $\rho^{(R)}_{ij}(t)$ (2) at T=0. Final and equilibrium values do not coincide (*non-ergodic*). Inset a) depicts $B^{\max}_{CHSM}$ versus h for $\gamma = 0.5$ and different distances between spins $R = 1, 2, 3$ and ∞ (dotted line). Though no Bell violation is observed, $B^{\max}_{CHSM}$ exhibits a long range order. Inset b) depicts equilibrium nonlocality (upper curves) and concurrence (lower curves) measures versus h for $\gamma \in [0, 1]$. The isotropic case $\gamma = 0$ collapses to 2 for $h \geq 1$. See text for details.

where $\mathbf{T^{(R)}} = (T^{(R)}_{xx}, T^{(R)}_{yy}, T^{(R)}_{zz})$ and $\min_{xyz} \equiv \min\left(\left[T^{(R)}_{xx}\right]^2, \left[T^{(R)}_{yy}\right]^2, \left[T^{(R)}_{zz}\right]^2\right)$. Fig. 1 depicts the evolution of nonlocality (7) for the case $\gamma = 0.5$ and ($h_0 = 0.5, h_f = 0$). For $\gamma = 1$ (Ising) and ($h_0 = h_c, h_f = 0$) (7) would oscillate indefinitely. This nonlocality measure oscillates around a value distinct from the one expected. Just as in the case of the M_z in [12], or entanglement in the XY model [15] (as measured by the concurrence C), (7) does not reach its equilibrium value, which entails that nonlocality is also a non-ergodic quantity.

The equilibrium case ($h_f = h_0$) is considered in Fig. 1a. $B^{\max}_{CHSM}$ evolves for different configurations up to $R = \infty$ [12]. It is apparent that nonlocality exhibits a long range behavior, while C rapidly tends to zero [16]. Comparison with entanglement appears in Fig. 1b for all γ-anisotropies. The usefulness of (bi)entanglement between spins in the XY model is questioned in quantum information processing by the fact that the concomitant correlations never violate a Bell inequality ($B^{\max}_{CHSM} \leq 2\ \forall\, h, \gamma$).

All previous quantities are ultimately described in terms of several G_R, so that they all diverge at $h = 1$ in the same manner. Let us consider for simplicity $M_z(h) = \frac{1}{2}G_0 = \frac{\partial}{\partial h}\frac{1}{2\pi}\int_0^\pi d\phi[\gamma^2\sin^2\phi + (h-\cos\phi)^2]^{1/2}$. For $\gamma = 1$ we have $M_z(h) = \frac{\partial}{\partial h}\left(\frac{2(h+1)}{2\pi}E\left[\frac{2\sqrt{h}}{h+1}\right]\right) =$

$\frac{1}{2\pi}\left[\frac{h-1}{h}K\left(\frac{2\sqrt{h}}{h+1}\right)+\frac{h+1}{h}E\left(\frac{2\sqrt{h}}{h+1}\right)\right]$, where $K(E)$ is the complete elliptic integral of the first(second) kind. $\frac{d}{dh}M_z$ diverges logarithmically at $h=1$ following the divergence of K, and so does C and B^{max}_{CHSM}, including non-equilibrium ($t=\infty$) values. Therefore entanglement and nonlocality exhibit one additional feature beside non-ergodicity: they both signal the presence of a QPT at T=0.

Three qubits Nonlocality in the three qubit case is explored through the violation of the Mermin inequality [17]. The Mermin inequality reads as $Tr(\rho B_{Mermin}) \leq 2$, where B_{Mermin} is the Mermin operator

$$B_{Mermin} = B_{a_1a_2a_3} - B_{a_1b_2b_3} - B_{b_1a_2b_3} - B_{b_1b_2a_3}, \quad (8)$$

with $B_{uvw} \equiv \mathbf{u}\cdot\sigma\otimes\mathbf{v}\cdot\sigma\otimes\mathbf{w}\cdot\sigma$ with $\sigma=(\sigma_x,\sigma_y,\sigma_z)$ being the usual Pauli matrices, and $\mathbf{a_j}$ and $\mathbf{b_j}$ unit vectors in $\mathbb{R}^3$. Notice that GHZ states maximally violate the Mermin inequality. As usual, we will employ

$$Mermin^{\max} \equiv \max_{\mathbf{a_j},\mathbf{b_j}} Tr(\rho B_{Mermin}) \quad (9)$$

as a measure for the nonlocality of the state ρ.

The XY model is completely solvable, a fact that allows us to compute – as in the previous case of two sites – the reduced density matrix for three spins without the explicit construction of the global infinite state of the system. The reduced state of three spins reads as

$$\rho^{(a,b)}_{ijk} = \frac{1}{8}\left[\mathbb{I} + \sum_{u,v,w} T^{(a,b)}_{uvw}\sigma^i_u\otimes\sigma^j_v\otimes\sigma^k_w\right], \quad (10)$$

where $i<j<k$ indicate the positions of the three spins and $a=j-i, b=k-j$ their relative distances. $\{u,v,w\}$ denote indexes of the Pauli matrices $\{\sigma_0,\sigma_x,\sigma_y,\sigma_z\}$, and $T^{(a,b)}_{uvw} \equiv \langle\sigma^i_u\otimes\sigma^j_v\otimes\sigma^k_w\rangle_{ab}$. Similarly to the calculation of the two-spin correlations computed by Barouch *et al* [12], based in turn on the work by Lieb *et al* [11], we extend them to the three party case by using the well known Wick theorem in quantum field theory. Due to the symmetry of the XY model, some of them vanish. Furthermore, as far as nonlocality is concerned, among those correlations who survive only four of them contribute to (9), namely, $T^{(a,b)}_{xxz}, T^{(a,b)}_{zxx}, T^{(a,b)}_{zxx}$ and $T^{(a,b)}_{zzz}$. These three-spin correlation functions $T^{(a,b)}_{xzx}, T^{(a,b)}_{xxz}$ and $T^{(a,b)}_{zzz}$ are given by

$$\begin{vmatrix} G_{-1} & \dots & G_{-a+1} & G_{-a-1} & \dots & G_{-a-b} \\ \vdots & & \vdots & \vdots & & \vdots \\ G_{a-2} & \dots & G_0 & G_{-2} & \dots & G_{-b-1} \\ G_a & \dots & G_2 & G_0 & \dots & G_{-b+1} \\ \vdots & & \vdots & \vdots & & \vdots \\ G_{a+b-2} & \dots & G_b & G_{b-2} & \dots & G_{-1} \end{vmatrix}, \quad (11)$$

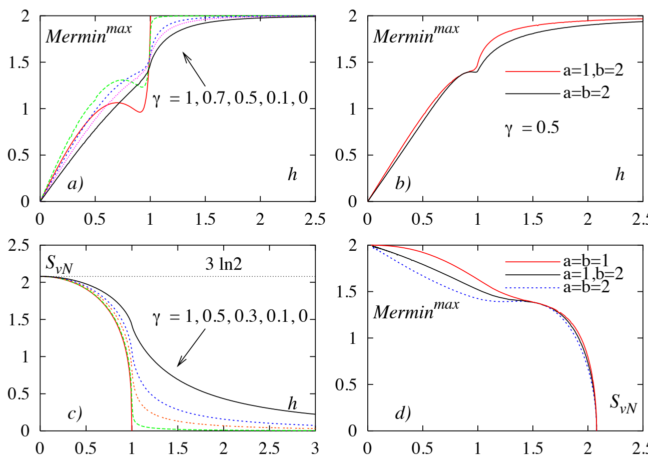

FIG. 2. (colour online). Fig. a) depicts the value of $Mermin^{\max}$ versus h (9) for several γ values for the $a=b=1$ block configuration. Fig. b) shows similar curves for $a=1,b=2$ and $a=2,b=2$, with $\gamma=0.5$. Fig. c) depicts the evolution of multipartite entanglement S_{vN} ($a=b=1$) versus h for several values of the anisotropy. Fig. d) plots $Mermin^{\max}$ versus S_{vN} for $\gamma=0.5$ and all previous configurations $a=b=1$, $a=1,b=2$ and $a=b=2$. Notice the apparent monotonic decreasing evolution. See text for details.

$$\begin{vmatrix} G_{-1} & \dots & G_{-a} & G_{-a-b} \\ G_0 & \dots & G_{-a+1} & G_{-a-b+1} \\ \vdots & \ddots & \vdots & \vdots \\ G_{a-2} & \dots & G_{-1} & G_{-b-1} \\ G_{a+b-1} & \dots & G_b & G_0 \end{vmatrix}, \begin{vmatrix} G_0 & G_{-a} & G_{-a-b} \\ G_a & G_0 & G_{-b} \\ G_{a+b} & G_b & G_0 \end{vmatrix} \quad (12)$$

respectively, with $T^{(a,b)}_{zxx} = T^{(b,a)}_{xxz}$ due to translational symmetry.

Correlations between parties strongly depend on their relative positions a and b. We shall distinguish two types: i) the one forming a block of three in consecutive sites ($a=b=1$), as well as a centered configuration ($a=b=2$), and ii) two nearest-neighbors spins plus an additional one ($a=1,b=2$).

Optimization of $Mermin^{\max}$ (9) for any configuration of the spins along the chain is carried out as follows. Once the observers' settings $\{\mathbf{a_j},\mathbf{b_j}\}$ are parameterized in spherical coordinates $(\sin\theta_k\cos\phi_k, \sin\theta_k\sin\phi_k, \cos\theta_k)$, the problem consists in finding the supremum of (9) over the set of $\{k=1..12\}$ possible angles. Here, too, we will consider ground state nonlocality.

Let us consider the block configuration $a=b=1$. The orientation of the settings $\{\mathbf{a_j},\mathbf{b_j}\}$ that maximizes $Mermin^{\max}$ (9) is such that ($x-z$ plane only, that is, we deal we *real qubits* for $u^y_j = 0\,\forall\mathbf{u}$) $\{\mathbf{a_3}=-\mathbf{a_1}, \mathbf{b_1}=\mathbf{a_2}, \mathbf{b_2}=-\mathbf{a_1}, \mathbf{b_3}=-\mathbf{a_2}\}$ for the whole range of h. Explicitly, $Mermin^{\max} = max_{\theta_{a_1},\theta_{a_2}}\left[a^z_2\left((a^z_2)^2 - 3(a^z_1)^2\right)T^{(1,1)}_{zzz} + \left(a^z_2\left((a^z_2)^2 - (a^x_1)^2\right) - 2a^z_1a^x_1a^x_2\right)\left(T^{(1,1)}_{zxx} + T^{(1,1)}_{xzx} + T^{(1,1)}_{xxz}\right)\right]$. The

ensuing analytic form of $Mermin^{\max}$ versus h – a complicated rational function with radicals– is calculated by recourse to convex optimization. For the sake of generality, let us also consider the centered configuration $a = b = 2$. After some algebra, we obtain that one disposition of the observers that provides an analytical expression for a lower bound to (9) is given by (again in the $x - z$ plane) $\{\mathbf{a_1} = (\sin\theta_{a_1}, \cos\theta_{a_1}), \mathbf{a_2} = (0,-1), \mathbf{a_3} = (\sin\theta_{a_1}, -\cos\theta_{a_1}), \mathbf{b_1} = \mathbf{a_3}, \mathbf{b_2} = (1,0), \mathbf{b_3} = -\mathbf{a_1}\}$. Hence, we obtain that $max_{\theta_{a_1}}\big[2\cos^2\theta_{a_1}T^{(2,2)}_{zzz} + 2\sin\theta_{a_1}\cos\theta_{a_1}T^{(2,2)}_{zxx} - 2\sin^2\theta_{a_1}T^{(2,2)}_{xzx} + 2\sin\theta_{a_1}\cos\theta_{a_1}T^{(2,2)}_{xxz}\big] \leq Mermin^{\max} \leq \sqrt{4\big(T^{(2,2)}_{zzz}\big)^2 + 4\big(T^{(2,2)}_{zxx}\big)^2 + 4\big(T^{(2,2)}_{xzx}\big)^2 + 4\big(T^{(2,2)}_{xxz}\big)^2}$. The analytic form of the lower bound – not provided here – is of the same nature of that of the $a = b = 1$ case. In point of fact, the lower bound becomes an equality for all (a, b) shortly before $h = 1$. Additionally, the upper bound also applies to all configurations.

Fig. 2a,2b present the situation, where $Mermin^{\max}$ is depicted for different values of the γ-anisotropy and different configurations of the spins. Numerical calculations perfectly agree with the corresponding analytic expressions. As h grows, the state $\rho^{(a,b)}_{ijk}$ approaches $|\downarrow\downarrow\downarrow\rangle\langle\downarrow\downarrow\downarrow|$ as expected (ferromagnetic phase), and *never violates the Mermin inequality*, which entails an inherent limitation to the usefulness of entanglement itself.

Characterization of entanglement is of paramount relevance in QIT [18], yet no operational measure is available to date that quantifies genuine multipartite entanglement. We will nevertheless employ the sum of the von Neumann entropy of the reduced density matrices of the three spins of $\rho^{(a,b)}_{ijk}$, $S_{vN} = 3S_{vN}(\rho_i)$, with $\rho_i = \frac{1}{2}(\mathbb{I} + \langle\sigma_z\rangle\sigma^i_z)$, $\langle\sigma_z\rangle = G_0 = 2M_z$. We shall consider ground state entanglement (T=0), as well. The specific form of S_{vN} is depicted in Fig. 2c for several values of the γ-anisotropy as a function of h. The monotonic decreasing tendency of entanglement is apparent for any γ-value. As h grows, the fidelity between $\rho^{(a,b)}_{ijk}$ steadily tends to 1.

Remarkably, we observe opposite tendencies revealed by entanglement S_{vN} and nonlocality (9). Recall that our model undergoes a second order QPT in the ground energy. In point of fact, since $\frac{d}{dh}S_{vN} \propto \frac{d}{dh}M_z$, this measure of multipartite entanglement (its derivative) diverges logarithmically at $h_c = 1$. Surprisingly, our measure of nonlocality (9) also displays such divergence, along with its bounds. In Fig. 2d we show the dependency of $Mermin^{max}$ versus entanglement S_{vN} for several values of γ in the $(a = 1, b = 1)$ configuration. Finally, we encounter for the first time a multipartite system where not only is entanglement (its first derivative) a good indicator of a QPT, but also nonlocality.

Conclusions We have studied how nonlocality – measured by the maximal violation of a Bell inequality– compares to entanglement in a condensed matter system. Although two instances (two and three sites) have been considered, our results may properly generalize to any block of spins. For the bipartite case, we have computed the exact value of $B^{\max}_{CHSM}$ during time evolution and in equilibrium. In either cases our nonlocality measure (7) displays a non-ergodic behavior, is able to detect a QPT, and limits the QIT-related tasks involving bipartite entanglement along the infinite chain since no Bell inequality is violated. A similar situation occurs in the tripartite case, where non-violation of local realism in the XY model takes place as well. Also, entanglement and nonlocality both indicate a QPT yet exhibit opposite evolutions in the phase diagram. Finally, nonlocality can also constitute a complementary resource in infinite quantum systems.

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